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A threshold line dissociation model for the direct simulation Monte Carlo method

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A new dissociation model for the direct simulation Monte Carlo (DSMC) method is formulated using the threshold line concept. This model considers in some detail the coupling between the vibrational energy distribution of molecules in a gas and the rate of dissociation. For a particular reaction, the new threshold line model only requires determination of a leading multiplicative constant and is therefore significantly less deterministic than existing DSMC chemistry models. The new model is evaluated in a heat bath under equilibrium and nonequilibrium conditions. It is also employed to calculate hypersonic shock waves of nitrogen and air. Comparison of the results generated with the new model is made with existing experimental data and with previous computational results. The more detailed DSMC implementation reveals properties of the threshold line dissociation model not apparent in the previous continuum implementation. © *1996 American Institute of Physics.* [S1070-6631(96)01005-3]

I. INTRODUCTION

In the present study we focus on the well-known mechanism whereby the rate of dissociation is altered under conditions of thermal nonequilibrium behind shock waves. Specifically, the dissociation rate is reduced when the vibrational temperature is lower than the translational value. This mechanism is often called coupled vibration dissociation (CVD). It is important to capture this phenomenon in computational models applied to high-temperature nonequilibrium flows. For example, in hypersonic flow of vehicles reentering the atmosphere of the earth, chemical nonequilibrium affects the heat load and pitching moment experienced by the body. In addition, the vibrational temperature is directly affected by the CVD model and this quantity is often used to estimate radiation emitted from hypersonic shock waves.

The two most popular approaches for performing numerical simulations of nonequilibrium flows are the various continuum based techniques of computational fluid dynamics (CFD), and the particle-based direct simulation Monte Carlo method (DSMC). In CFD methods, the continuum equations of fluid dynamics are solved using finite difference or finite volume formulations. In the DSMC technique, a direct simulation of the gasdynamics is performed using particles that move in physical space and undergo intermolecular collisions. Clearly, with the DSMC approach, there is the opportunity to include more detailed physics for collision phenomena. Unfortunately, this more direct approach is more numerically intensive limiting application of the DSMC technique to flows of relatively low density (e.g., Knudsen numbers larger than 10^{-4}).

Several CVD models have been proposed over the years for both CFD and DSMC simulations.[1-6] The models most frequently employed in large-scale numerical simulations of nonequilibrium flows are highly phenomenological. The goal of this paper is to investigate use of a more detailed, less phenomenological CVD model for the DSMC technique. The approach adopted is to use the threshold line concept employed by Macheret and Rich[4] to derive a continuum CVD model. The development of such a model for the particle DSMC technique requires adaptation of the threshold line method to a detailed microscopic kinetic theory analysis. It will be shown that this analysis reveals features of the threshold line concept not previously apparent through the continuum analysis of Ref. 4.

The outline of the paper is as follows. First, the standard CVD models are described for flow simulations based on continuum and particle representations of the fluid. Then, the continuum CFD model proposed by Macheret and Rich[4] that is based on the threshold line concept is introduced. In the present study, based on work of Macheret *et al.*,[5] a threshold line model suitable for the particle approach is considered. Basic properties of the model are investigated under equilibrium and nonequilibrium conditions. Results obtained with the new model are compared with experimental measurements in hypersonic shock waves of nitrogen and air.

II. CVD MODELS

As mentioned previously, a number of models for simulating the coupling between the distribution of vibrational energy and the dissociation rate have been proposed. Some of the more popular models are described in Refs. 1–6. Of these, all but that of Boyd[6] are based on continuum formulations. In the following, the CVD models presented in Refs. 2 and 6 are described in detail due to their relatively widespread use in continuum and particle simulations of nonequilibrium flows.

A. Continuum approach

In continuum computational fluid dynamics (CFD), the two-temperature model of Park[2] is widely used. In this model, an Arrhenius reaction rate coefficient has its temperature dependence governed by

$$T_a = T_t^s \times T_v^{1-s},$$ (1)

where T_t is the translational temperature, T_v is the vibrational temperature, and s is a modeling parameter. This model is basically empirical but has enjoyed a fair degree of success. It is clearly phenomenological in that it retains equilibrium behavior when the translational and vibrational temperatures are equal and results in a reduction of the dissociation rate when the vibrational temperature is less than the translational value. The value of the parameter s is usually set to 0.5 for dissociation of molecular nitrogen and oxygen. As an indication of the empiricism involved with the model, however, some studies have recommended use of a value of 0.7.[7] The basic failing of the model is that there is no way to determine an appropriate value for s except through direct comparison with experimental data.

B. Particle approach

In the particle-based direct simulation Monte Carlo (DSMC) method, the vibrationally favored dissociation (VFD) model proposed in Refs. 6 and 8 is considered. In this model, the probability that a particular collision of two particles leads to dissociation is given by

$$P_d = f(E_c) \times E_v^\phi, \tag{2}$$

where $f(E_c)$ is a function of the total collision energy, E_c; E_v is the vibrational energy; and ϕ is a modeling parameter. The total collision energy is the sum of the translational, rotational, and vibrational energies of the colliding particles. In Refs. 6 and 8, it has been determined empirically through comparison with experimental data that appropriate values for the parameter ϕ are 2 for nitrogen, and 0.5 for oxygen. The mathematical form for this model is based on analytical convenience rather than physical behavior. By including the additional term, in which the vibrational energy is raised to the power ϕ, coupling between vibrational energy and dissociation rate is included at a simple level. Particles with higher vibrational energies produce higher probabilities of dissociation than lower lying particles. At the macroscopic level, the model produces the desired CVD behavior, in that when the vibrational temperature is less than the translational temperature, the dissociation rate is reduced below its equilibrium value.

As with the Park model for continuum simulations, the disadvantages of the VFD model are its high degree of empiricism and the fact that there is no systematic way to determine ϕ for each new species of interest.

III. THRESHOLD LINE MODELS

The threshold line concept is based on the premise that a certain amount of translational energy in a collision is required above the vibrational energy of the molecule to effect the dissociation reaction. This required energy is the threshold, F. While the model is developed from a collisional standpoint, emphasis has been placed in Refs. 4 and 5 on continuum forms of the model. In the following sections, both continuum and particle forms of the threshold line concept are discussed.

A. Continuum approach

In the work of Macheret and Rich,[4] it is proposed that at high vibrational energy levels the threshold energy is simply the difference between the activation energy of the reaction and the molecular vibrational energy. By detailed consideration of the collision dynamics involved in the dissociation process, it is proposed that the threshold energy at low vibrational levels is larger than this simple difference.

Using these ideas, continuum models expressed in terms of translational, rotational, and vibrational temperatures have been proposed by Macheret et al.[5] to model nonequilibrium dissociation processes. Current interest in the threshold line concept has arisen in part from the successful application of the continuum-based model of Ref. 4 by Boyd et al.[9] In this study, the threshold line model gave the first successful predictions of data from a high-altitude, hypersonic flight experiment.

The continuum models presented in Refs. 4 and 5 are based on integration of collision probabilities over equilibrium energy distributions. To obtain analytical results, it was necessary in these studies to employ approximations in this integration process. Specifically, the method of steepest descent and a continuous form of the vibrational energy distribution were employed.

A key point about the continuum threshold line models is the manner in which their behavior is constrained under equilibrium conditions. The approach adopted is to ensure, when all the temperatures are equal, that the rate coefficient provided by the model corresponds to the modified Arrhenius form:

$$k_d = aT^\eta \exp(-D/kT), \tag{3}$$

where a and η are constants, k is the Boltzmann constant, and D is the activation energy of the reaction. Hence, the constants a and η appear directly in the continuum versions of the threshold line model. One subtle effect of imposing this condition on the model is that a specific temperature dependence is being imposed on the probability of reaction. This approach is not applicable to the particle method that requires dissociation probabilities to be described purely in terms of collision energies as described in the following section.

B. Particle approach

The purpose of this study is to use the threshold concept to develop a nonequilibrium dissociation model that may be employed directly in the DSMC technique. This requires the formulation of a dissociation probability based on the translational collision energy and the rotational and vibrational energies of the dissociating molecule. This has been performed in the work of Macheret et al.[5] However, the final results of that study are described in terms of continuum temperatures rather than collision energies. For simplicity, the following discussions will be concerned with dissociation of molecular nitrogen through collisions with other nitrogen molecules or atoms.

As described in detail in Ref. 5, the threshold line probability of dissociation has distinct mathematical forms for

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low and high vibrational levels. At low vibrational levels, there is insufficient velocity along the line of centers of the two atoms that constitute the molecule to match the translational velocity of the colliding atom. This is the requirement that must be met to allow all of the translational energy of the atom to be transferred into the vibrational energy of the molecule and thus cause dissociation. Hence, at low vibrational energies, the threshold energy required to cause dissociation is greater than the difference between the activation energy and the translational collision energy. As proposed in Ref. 4, the boundary between high and low vibrational levels is determined using the following parameter:

$$\alpha = \left(\frac{m}{m+M} \right)^2,$$ (4)

where m is the mass of one of the two atoms in the diatomic molecule that is dissociating, and M is the mass of the collision partner. In the case of diatom–diatom collisions, M is the mass of one of the atoms in the second molecule, and therefore α is equal to 0.25 for both N_2–N_2 and N_2–N collisions.

In the following expressions, E_t is the translational collision energy, and E_r and E_v are the rotational and vibrational energies of the reacting molecule. In this study, the vibrational energy distribution is modeled as a simple harmonic oscillator using the approach of Bergemann and Boyd.[10] The threshold line model specifies low vibrational energy levels as those for which $E_v < \alpha D^*$, where D^* is a modified activation energy that will be defined later. Using these ideas, it may be shown[11] that the dissociation probability of low vibrational levels for diatom–atom collisions is

$$P_d = A_i \frac{8\sqrt{2}(E_t - F)^{3/2}}{3\pi^2 F[(\sqrt{D^*} - \sqrt{\alpha E_v})[\sqrt{D^*} - (2-\sqrt{\alpha})\sqrt{E_v}]]^{1/2}},$$ (5)

where A_i is a constant of proportionality for reaction i that does not appear in the continuum formulation. It is necessary here in order to calibrate the DSMC model against specified rate coefficients. In the continuum model, A_i has some unknown functional form that ensures the Arrhenius rate coefficient is recovered at equilibrium. For low vibrational levels, the threshold energy is given as

$$F = \frac{(\sqrt{D^*} - \sqrt{\alpha E_v})^2}{1-\alpha}.$$ (6)

At high vibrational levels ($E_v > \alpha D^*$), the threshold energy is simply

$$F = D^* - E_v.$$ (7)

Following the procedures outlined in Ref. 5, the dissociation probability at the high vibrational levels for diatom–atom collisions is derived here as

$$P_d = A_i \sqrt{\frac{1+\sqrt{\alpha}}{1-\sqrt{\alpha}}} \frac{(E_t - F)^2}{4\pi^2 F^{3/2}\sqrt{E_v - \alpha D^*}},$$ (8)

where the constant of proportionality A_i is the same as that in Eq. (5).

The participation of rotational energy in the reaction process is included by proposing an effective activation energy of the form[5]

$$D^* = D - E_r + \frac{2E_r^{3/2}}{3\sqrt{6D}},$$ (9)

where D is the dissociation energy. At very high rotational energies, the activation energy is reduced due to the strong centrifugal force induced on the molecule. This aspect of the model reduces the dissociation rate in comparison with the equilibrium value when the rotational temperature is less than the translational value. This effect is much smaller than the coupling with the vibrational energy mode.

In Ref. 5, separate threshold line models are presented for diatom–diatom and diatom–atom collisions. In the present study, however, the above probability model (strictly valid only for diatom–atom collisions) is employed for both N_2–N_2 and N_2–N dissociation reactions. This approach is adopted due to the requirement for a relatively simple mathematical expression for use in the numerically intensive DSMC technique.

As with the continuum model, the particle based threshold line probability must at the macroscopic level recover a specified Arrhenius rate coefficient under equilibrium conditions. Unlike the continuum model, however, the Arrhenius constants a and η do not appear in the model. Instead, the constant of proportionality, A_i, must be obtained through calibration of the model against rate data by performing test simulations under equilibrium conditions. Hence, with this approach, it is not possible to guarantee that the model will produce a specific temperature dependence for the dissociation rate. This could perhaps be achieved through inclusion of further dependencies of the dissociation probability on the various energies involved in the collision. This lies beyond the scope of the present study.

IV. RESULTS

The properties of the threshold line dissociation model for the DSMC technique are first assessed in simple heat bath conditions. These are used to calibrate the model against experimental measurements of dissociation rate coefficients. In addition, comparison of the DSMC model with the continuum threshold line model is conducted. The calibrated DSMC models are then applied to normal shock waves of nitrogen, and to a bow shock wave in air. In the latter cases, direct comparison of simulated results with available experimental data is undertaken.

A. Equilibrium heat bath

The DSMC threshold line model is used to calculate dissociation rate coefficients under conditions where the translational, rotational, and vibrational modes are in thermal equilibrium with Boltzmann distributions. An isothermal heat bath is simulated that consists of 50 000 particles. Energy is exchanged between the various modes during collision, but chemical reactions are not processed. Instead, the average dissociation probability is evaluated over all collisions and then converted into a rate coefficient. Results ob-
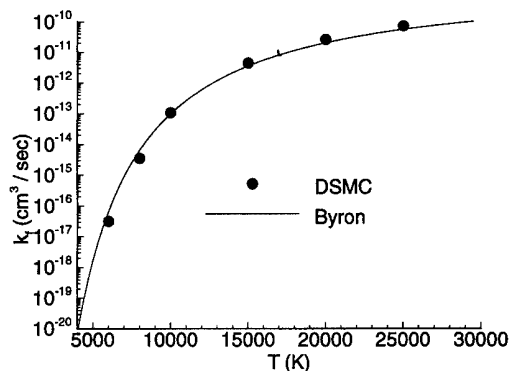
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FIG. 1. Dissociation rate coefficient for N_2-N_2 under conditions of thermal equilibrium.

tained in this manner are compared in Fig. 1 over a wide temperature range with the following rate coefficient of Byron[12] for the N_2-N_2 reaction:

$$r_{N_2-N_2} = 7.97 \times 10^{-7} T^{-0.5} \exp(-113\,200/T).$$

The units are $cm^3/mol/s$. As discussed by Boyd,[6] the data of Byron are employed as they were measured under conditions of thermal equilibrium. It is quite remarkable that the DSMC model provides a temperature dependence that is so close to the Byron rate. It should be noted that the leading constant in the DSMC model is explicitly chosen to give agreement with the Byron rate at $T = 10\,000$ K. In this case, $A_{N_2-N_2} = 5$.

In Fig. 2 the dissociation probabilities predicted by the model for N_2-N_2 collisions at several different vibrational energy levels are plotted as a function of translational collision energy (expressed as a temperature by dividing by $2k$). It is interesting to note that there is a region for all vibrational levels where the dissociation probability exceeds unity. In practice, when using a probability model in a DSMC calculation, the reaction rate simulated will employ a maximum reaction probability of unity. That is, even if the reaction probability is equal to 2.0, only one reaction is processed. Thus, the dissociation rates shown in Fig. 1 were generated by limiting the dissociation probability to a maximum of unity.
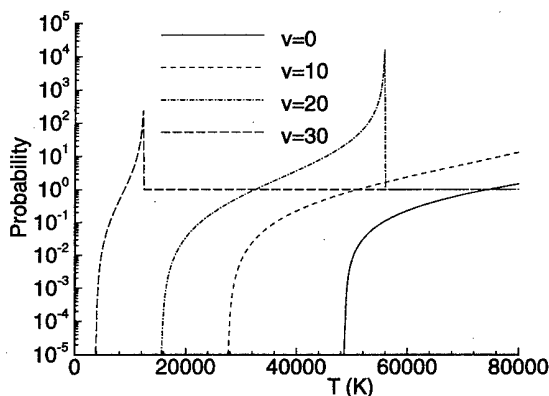

FIG. 3. Dissociation rate coefficient for N_2-N under conditions of thermal equilibrium.

The behavior of the DSMC model for N_2-N collisions is shown in Fig. 3. In this case, the selection of rate data is more difficult. The rate coefficients considered for this reaction are those reported by Byron[12] as

$$r_{N_2-N} = 7.17 \times 10^{-2} T^{-1.5} \exp(-113\,200/T),$$

by Cary[13] as

$$r_{N_2-N} = 2.71 \times 10^{-4} T^{-1.0} \exp(-113\,200/T),$$

and by Flagan and Appleton[14] as

$$r_{N_2-N} = 2.76 \times 10^{-2} T^{-1.6} \exp(-113\,200/T).$$

In all cases the units are $cm^3/mol/s$. The DSMC results are obtained using a leading constant in the threshold line model of $A_{N_2-N} = 14$. Good agreement is found with Refs. 13 and 14 at low temperature, and better agreement with Ref. 12 at high temperature.

Results for O_2-O_2 and O_2-O dissociation reactions are shown in Figs. 4 and 5, respectively. The Arrhenius rates in each case are those reported by Byron:[15]

$$r_{O_2-O_2} = 3.27 \times 10^{-3} T^{-1.5} \exp(-59\,400/T)$$

FIG. 2. Probability of dissociation at various vibrational energy levels as a function of translational collision energy for the N_2-N_2 reaction.
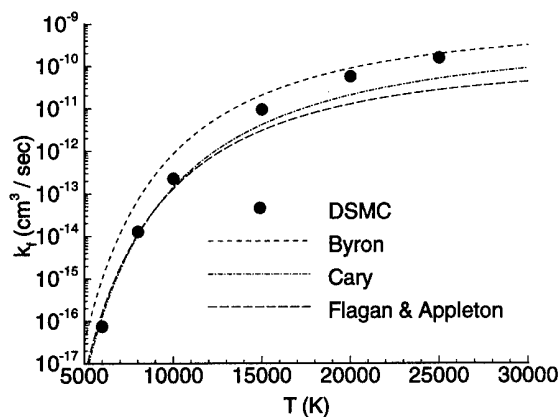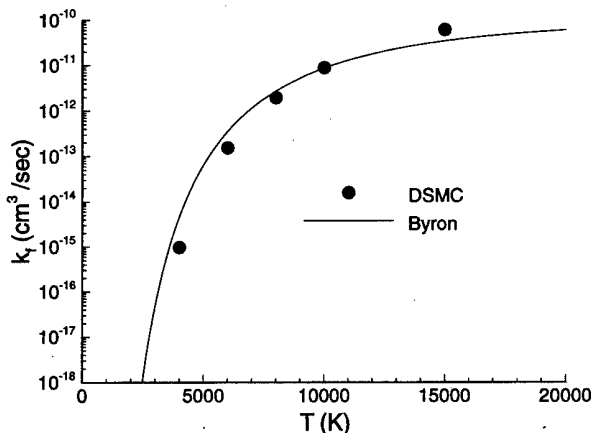

FIG. 4. Dissociation rate coefficient for O_2-O_2 under conditions of thermal equilibrium.
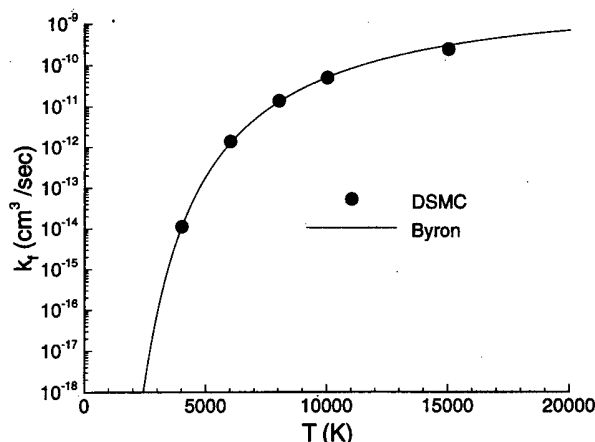
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FIG. 5. Dissociation rate coefficient for O_2-O under conditions of thermal equilibrium.

and

$$r_{O_2-O} = 1.95 \times 10^{-6} T^{-0.5} \exp(-59\,400/T),$$

where the units are $cm^3/mol/s$. The threshold line model is calibrated for each reaction at a temperature of 10 000 K, giving leading constants of $A_{O_2-O_2} = 1.25$ and $A_{O_2-O} = 32$. Consistent with the results obtained for nitrogen dissociation, the DSMC threshold line model for oxygen gives better agreement with an Arrhenius rate coefficient having a temperature exponent of -0.5.

The key aspect of all CVD models is the manner in which molecules are selected preferentially for dissociation based on their vibrational energy. Further equilibrium simulations are performed to analyze how this occurs at the collision level in the threshold line model. Once again, several million collisions are simulated using 100 000 particles in equilibrium at 10 000 K. Using an accept–reject approach, individual collisions that give rise to dissociation are identified. For each of these reactive collisions, the vibrational energy of the reacting molecule is recorded. The vibrational energy distributions of reactive molecules obtained in this manner with the threshold line and VFD dissociation models for N_2-N_2 collisions are compared in Fig. 6. The distributions produced by the two models are very different. By
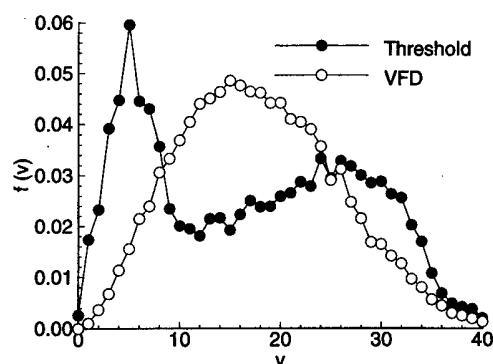

FIG. 6. Distribution of vibrational energy for reacting nitrogen molecules under equilibrium conditions at 10 000 K.
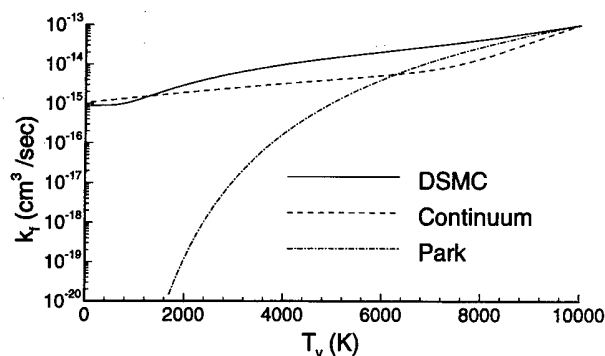

FIG. 7. Dissociation rate coefficient for N_2-N_2 as a function of vibrational temperature at $T_t = T_r = 10\,000$ K.

comparison with the VFD model, the threshold line model dissociates many more molecules at low vibrational levels. This is a significant effect that will become important in nonequilibrium flow conditions. Note that the border between low and high vibrational levels in the threshold line model occurs for N_2 at a vibrational quantum number of 8. At this point, the vibrational energy distribution of reacting molecules undergoes a distinct but smooth change in profile. While the minimum in the vibrational energy distribution of reacting particles shown in Fig. 6 is an interesting property of the model, it is not, unfortunately, feasible to measure this energy distribution experimentally.

B. Nonequilibrium heat bath

Comparison is next made of the DSMC threshold line model with the continuum model of Macheret et al.[5] under nonequilibrium conditions. For simplicity, the translational and rotational modes are equilibrated. Only the effect of vibrational nonequilibrium is considered. Once again, heat bath simulations are performed. In this case, the translational and rotational modes are given a temperature of 10 000 K. For each of the vibrational levels of the harmonic oscillator that lie below the dissociation energy, a large number of collisions are calculated to determine the state-dependent dissociation rate. These rates are then summed over the Boltzmann populations at different vibrational temperatures. The results of this analysis are shown in Fig. 7 for the N_2-N_2 reaction. Comparison is made with the continuum threshold line model. For reference, the dissociation rate produced by the Park model using $s=0.5$ is also shown. This illustrates the key aspect of the threshold line models, which is that they predict substantially higher dissociation rates under conditions of strong thermal nonequilibrium.

Concentrating on the two threshold line profiles in Fig. 7, it is seen that they give good agreement at the lower and upper values of vibrational temperature. However, the DSMC model predicts a higher dissociation rate for the intermediate values. The reason for this difference is partly explained through consideration of Fig. 8. This shows the contributions to the overall dissociation rate of the lower $(E_v < \alpha D)$ and higher $(E_v > \alpha D)$ vibrational levels. The DSMC model generally shows higher dissociation rates from
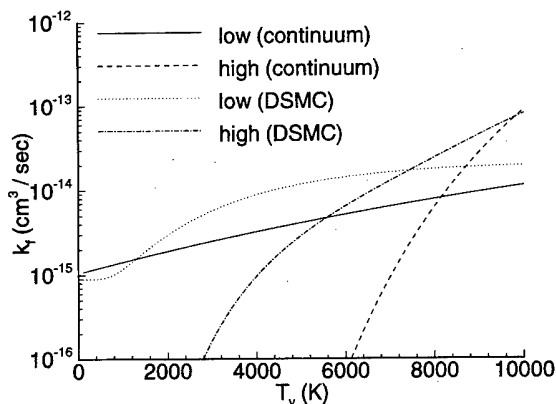
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FIG. 8. Contributions of high and low vibrational levels to the dissociation rate coefficient for N_2–N_2 as a function of vibrational temperature at $T_t = T_r = 10\,000$ K.

FIG. 9. Ratio of local to upstream density in a hypersonic shock wave of nitrogen: $U_1 = 4.8$ km/s.

both low and high vibrational levels. It is assumed that these differences arise from the approximations made in obtaining analytical expressions for the continuum model. In particular, integrals are evaluated using the method of steepest descent, which can give rise to significant inaccuracies. In addition, the continuum model assumes a continuous distribution of vibrational energy whereas the DSMC approach employs the truncated harmonic oscillator.

C. Normal shock waves of nitrogen

In this section, the DSMC threshold model is evaluated through direct comparison of results obtained with the threshold line models and existing experimental data for hypersonic shock waves of nitrogen. The data is taken from Kewley and Hornung,[15] who report density profiles obtained from interferograms. Two cases with different upstream velocities are considered. The DSMC simulations of these one-dimensional shocks employ several thousand cells and about 100 000 particles. In the first case, the upstream velocity and density are 4.8 km/s and 4.67×10^{-2} kg/m^3, respectively. These conditions give a post-shock mole fraction of atomic nitrogen of just 0.15. Thus, for this case, the density profile is primarily characterized by N_2–N_2 dissociation reactions. The DSMC results computed with the threshold line model compare very favorably with the experimental data, as indicated in Fig. 9. The second case considers an upstream velocity and density of 7.3 km/s and 7.48×10^{-3} kg/m^3, respectively. Under these more energetic conditions, the post-shock mole fraction of atomic nitrogen is 0.60. Thus, in this case, the density rise across the shock is dominated by N_2–N dissociation reactions. The profile obtained with the threshold line model is compared with the experimental data in Fig. 10. Once again, good agreement is obtained between simulation and measurement. The level of agreement obtained with the threshold line models and the experimental data shown in Figs. 9 and 10 is nearly identical to that reported in Ref. 6 for the VFD chemistry model. It should be noted, however, that the agreement for the VFD model was only obtained through appropriate selection of the phenomenological parameter ϕ in Eq. (2).
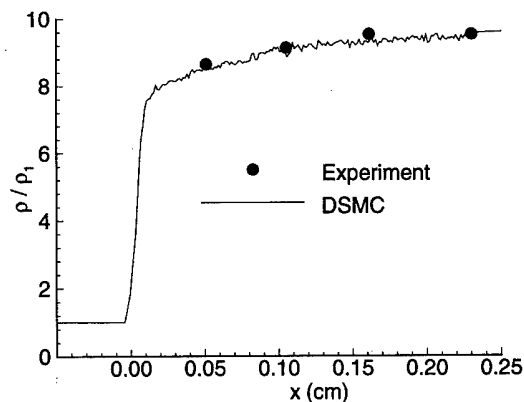
D. Bow shock wave of air

To evaluate the threshold line models for oxygen dissociation, the BSUV-2 flight experiment is considered. As mentioned earlier, favorable comparisons of results obtained with the continuum threshold line models and experimental data from this flight were reported in Ref. 9. The solutions at the highest altitudes considered at 85 and 88 km were obtained in Ref. 9 using a two-step process. First, a DSMC solution of the flow field was generated that considered only the major species of N_2 and O_2. Using this as input, the species conservation equations were then solved for the minor species of NO, N, and O with a finite volume overlay technique. Within this continuum overlay scheme, production of atomic nitrogen and oxygen through dissociation reactions was modeled using the continuum threshold line model of Macheret and Rich.[4] An overlay approach is appropriate, as the concentrations of the minor species are several orders of magnitude lower than those of the major species.

In the present work, the particle threshold line models for dissociation of nitrogen and oxygen are applied to the flow field generated by the BSUV-2 vehicle at a velocity of 5.1 km/s and an altitude of 85 km. The geometry is approximated by the front portion of a sphere of radius 10 cm rep-
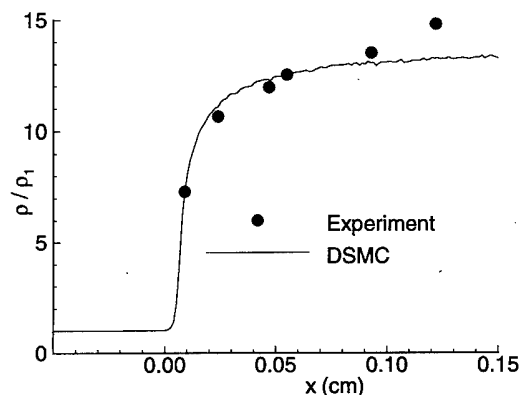

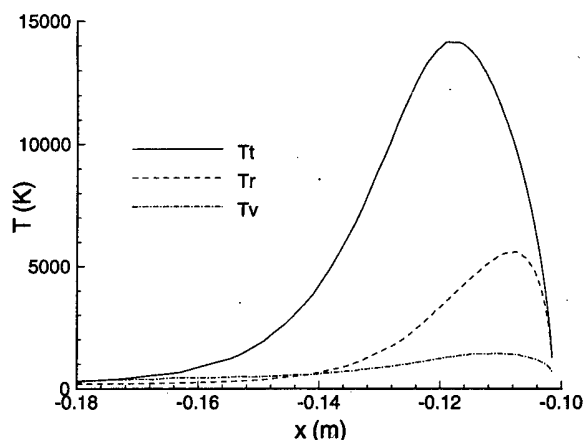FIG. 10. Ratio of local to upstream density in a hypersonic shock wave of nitrogen: $U_1 = 7.3$ km/s.

FIG. 11. Temperatures along the stagnation streamline of BSUV-2 at 85 km altitude.

resenting the nose of the vehicle. The temperature profiles for the translational, rotational, and vibrational modes along the stagnation streamline for this case are shown in Fig. 11. Clearly, a very strong degree of thermal nonequilibrium exists. In Fig. 12, concentrations of atomic oxygen and nitric oxide along the stagnation streamline are shown. Results obtained previously using the continuum threshold line model in the continuum overlay scheme (MR-CFD) are compared with those computed using the particle models presented earlier in this study (MR-DSMC). Excellent agreement is obtained for the two solutions. In the present study, the DSMC computation of these minor species is handled directly, without the need for an overlay computation using a weighting scheme, and this accounts for the statistical scatter seen particularly in the NO results. The agreement obtained is significant, as the previous continuum results provided excellent agreement with experimental measurements of radiative emission of both atomic oxygen and nitric oxide, as reported in Ref. 9.

V. CONCLUDING REMARKS

A threshold line dissociation model for the DSMC technique has been formulated that determines the probability of reaction based on the energy of each collision. For a particular dissociation reaction, the model only requires determination of a leading constant through comparison with an Arrhenius rate coefficient. The model was found to reproduce the temperature dependence of measured rate data under equilibrium conditions. In agreement with the original continuum threshold line model, the new particle-based threshold line model predicted dissociation rates under conditions of strong thermal nonequilibrium that are orders of magnitude higher than those predicted by existing dissociation coupling models. In application of the new model to hypersonic shock waves of nitrogen, excellent agreement was obtained with experimental measurements of density. For hypersonic, dissociating air at high-altitude conditions, the new models for nitrogen and oxygen dissociation were applied and found to give excellent agreement with previous computational results obtained with the continuum threshold line model.

An additional aspect of the DSMC implementation of the threshold line concept for dissociation was that properties of the model were revealed that were not apparent from the previous continuum implementation. First, a minimum in the vibrational energy distribution of dissociating molecules was obtained. Second, the rate of dissociation under thermal nonequilibrium conditions was found to reach an asymptotic value as the vibrational temperature tended to zero.

These studies have demonstrated the physical accuracy of the threshold line models presented in this investigation, and their use is recommended over previous phenomenological DSMC models for vibration–dissociation coupling.
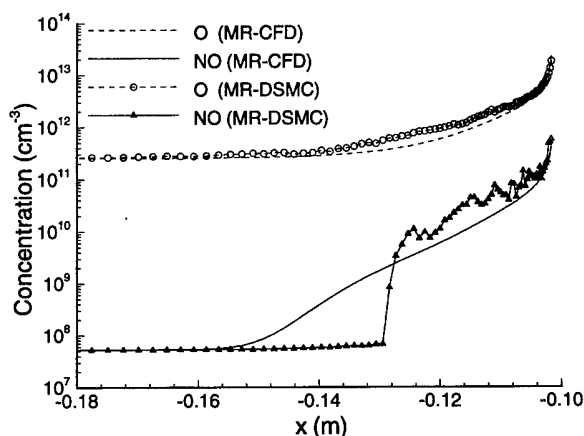
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FIG. 12. Concentrations of atomic oxygen and nitric oxide for the stagnation streamline of BSUV-2 at 85 km altitude: Comparison of current DSMC results with CFD overlay results of Ref. 9.

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